Analysing and Calculation
of Macrosegregation in a Casting Ingot. A MPS
Solidification Model, Volume 3: Operating
Manual Final Report (General Electric Co.)

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SECTION 1 - INTRODUCTION

This volume describes the operation of solidification model 1 using the Prime 400 computer system at MSFC. Model 1 calculates the macrosegregation in a rectangular ingot of a binary alloy as a result of horizontal axisymmetric bidirectional solidification. The calculation is restricted to steady-state solidification; there is no variation in final local average composition in the direction of isotherm movement. A description of the physics of the model is in Volume I of this report.

The solidification program allows interactive modification of calculation parameters as well as selection of graphical and tabular output. In batch mode, parameter values are input in card image form and output consists of printed tables of solidification functions. Both modes of operation are explained below, with the mechanical details related to use of the computer system separated from the specific details of the model parameters. This manual documents only the operation of the program; documentation of the FORTRAN program is in Volume II of this report. The input parameters in Sections 5 and 6 and the output selections in Section 7 are described in terms of the symbolism and terminology of Volume I.
SECTION 2 - COMMUNICATING WITH THE PRIME

Interactive communication between the Prime 400 and the user is effected by the Tektronix 4014 CRT (cathode-ray tube) terminal. The Prime displays messages and graphical representations on the screen, and the user sends commands or data to the Prime by typing them on the Tektronix 4014 keyboard. The items below describe some less obvious aspects of operating the terminal as well as some conventions used in communicating with the system.

2.1 ENTERING INFORMATION
The Tektronix 4014 keyboard is similar to the keyboard of an electric typewriter, with three notable exceptions. The numeral one is distinguished from the lower case letter "l". The RETURN key operates as a send key: to transmit data or a command to the Prime, type the text and then push RETURN. In all examples shown in this manual the use of the RETURN key is implicit. There is no backspace capability. Typing errors can be corrected, before pushing RETURN, by typing one " (shift 2) for each character in error. For example, "1234" would be sent as 1256.

2.2 NUMBERS
The FORTRAN form of scientific notation uses an E to separate the power of ten from the mantissa. Thus,

\[ .0001234 \text{ is written } 1.234\times10^{-4} \]

All numerical input to the program is handled by a FORTRAN feature known as "list-directed input". Although this is the least restrictive method available in the FORTRAN language, there are some limitations the user should note. Embedded blanks in a number will cause undesirable results, for example, 12 34. would be interpreted as 12., and 1.234 E3 would be interpreted as 1.234

Furthermore, a null input or an entirely blank input will be ignored, and the program will wait for another user response.
2.3 INTERRUPT KEY

Under normal circumstances the user will terminate operation of the program by selecting the Q option while in the output phase described in Section 3.5. However, it is possible to interrupt the execution of any user program at any time by pushing the BREAK key once. The system will respond immediately with the message "QUIT". The user should then send the command

```
C ALL
```

At this point the terminal is under control of the Prime system monitor in the same state as that after a `LOGIN`.

2.4 HARD COPY

To obtain a permanent copy of any display on the screen, push the "COPY" switch located at the upper right corner of the Tektronix console. A vertical line will move across the screen from left to right. Shortly after it passes off the screen the copy will appear in the tray of the adjacent hard copy unit.

2.5 BLANK DISPLAY

If the information on the screen is static for longer than 90 seconds, the display will be blanked out. This is a protective mechanism within the Tektronix terminal which prolongs the life of the CRT. To restore the display, push a SHIFT key. To clear the screen at any time, push the PAGE key.

2.6 SPEED OF RESPONSE

The length of the delay between sending any command and getting back the result will vary from session to session depending on the total number of users on the Prime system and the types of programs they are running.
SECTION 3 - RUNNING THE MODEL IN INTERACTIVE MODE

A typical interactive session consists of logging in to the Prime 400 system, invoking execution of the solidification program, running one or more cases, and logging out. The mechanical details of this process are described below.

3.1 LOG-IN PROCEDURE

To initiate any interactive session the user must identify himself to the Prime with a valid user "name". This is accomplished by sending the command

`LOGIN MPS`

where "MPS" is the name under which the materials processing programs are stored. The system responds with a message acknowledging the LOGIN, and it is ready to accept a command after it displays the message "OK,"

3.2 STARTING THE SOLIDIFICATION MODEL

After logging in, the user initiates execution of the program by entering two commands. The first is

`CO MPS1`

The Prime will put several messages on the screen, the last of which are

```
OK, CO -END
OK,
```

The Prime is then ready for the second command:

`SEG #MPS1`

The model identification page will appear on the screen shortly after this message is sent.

3.3 INPUT PHASE

For each case, the program passes through three phases of operation. The first is the input phase during which the user defines the case to be run by specifying the case title, the binary alloy and the values of the model parameters. At each step the program clearly specifies the type of information it requires. The code is able to trap and recover from input errors, thus avoiding fatal FORTRAN I/O errors which would necessitate restarting the program. The input parameters are defined in a later section. Each time execution is initiated

3-1
the built-in default case will appear in the model. If any parameter is changed during the input phase, the new value will remain in effect through subsequent cases in the same session or until it is changed again. Copies of the input phase displays are shown in the examples section. Some operational notes for each step of the input phase follow.

- The case title is simply typed in; if none is desired, push RETURN.
- The solvent and solute are entered as (uppercase) chemical symbols with no leading or embedded blanks. The program then checks the alloy data base, and if the data for the requested alloy is found, it is displayed on the screen. If the alloy is not in the data base, an error message and a list of alloys in the data base are displayed, and the user is allowed to select another alloy. Figure 3.1 shows the appearance of the display in the error situation.
- The remaining parameters are grouped under several broad classifications; each group is a separate display page in the input phase. When a parameter is changed, the display is refreshed with the new value. The user can change any, all, or none of the parameters in a group before proceeding to the next group. An example of the error-trapping mechanism for this type of input is shown in Figure 3.2.

3.4 CALCULATION PHASE

After the last group of input parameters is completed, the model enters the second stage of operation, the calculation phase. During this phase, the program determines the numerical solution to the equations describing the model subject to the conditions defined by the input parameters. There is no user interaction during the calculation. The message "calculation in progress" is put on the screen, and after each iteration on the nonlinear system (see Volume 1) the maximum relative change in $g_L$ is displayed as an aid in monitoring the progress of the solution. When the calculation is complete, the terminal bell rings and the operation of the program enters the output phase.

3.5 OUTPUT PHASE

The three levels of operation during the output phase are illustrated in Figure 3.3. At the highest level the user can choose to display graphical
The only Al-Cu system in the data base used here is limited to alloys below 33% Cu.

The user decides to process Al-15% Cu.

Figure 3.1. Alloy Selection Error Display

Figure 3.2. Parameter Group Error Display
ENTER T TO DISPLAY TABULAR DATA, G TO DISPLAY GRAPHS, Q TO TERMINATE RUN, OR N TO PROCEED TO NEXT CASE.

CALCULATION PHASE

ENTER ITEM NUMBER OF FUNCTION TO PLOT, OR P TO PROCEED

FUNCTION TO PLOT
1. COMPOSITION
2. VELOCITY

ENTER ITEM NUMBER OF PLOT TYPE
1. VERTICAL PROFILES

Figure 3.3. Levels of Operation During Output Phase
output, to display tabular output, to terminate execution of the program, or
to terminate the case by proceeding to the next case.

- At the graphical output level the user is given a choice of functions to plot
  and types of plot to use as shown in example 8.1.1. Immediately after entry
  of the plot type, the plot will be generated on the screen*. When the cursor
  remains motionless at the upper left corner of the screen, the plot is
  complete. To leave the plot display and return to plot selection mode,
  enter a P.

- At the tabular output level the display commences immediately after user
  selection of a function. Each time the screen is filled, the program waits
  for the user to enter a P before proceeding to the next display page or
  to the function selection page. On a typical 20 X 20 mesh a scalar function
  such as g, requires only one page while a vector function such as velocity
  requires three pages.

- Note that it is possible to switch freely between graphical and tabular
  output at the highest control level.

- After entering a Q to terminate execution or an N to proceed to the next
  case, the user can return to output mode only by re-running the case.

3.6 LOG-OUT PROCEDURE

It is possible to log out of the system only while the terminal is under the
control of the Prime monitor. The user exits the solidification program and
returns control to the Prime monitor either by entering a Q during the highest
level of the output phase or by following the interrupt procedure described
in Section 2.3. To log out enter

LO

*In the case of macrosegregation profiles, the user is given the opportunity
to override the computed scale with an input scale.
SECTION 4 - RUNNING THE MODEL IN BATCH MODE

The term "batch" describes a program in which the user prescribes values for all input parameters before the execution begins, and output is available to the user only after execution is completed. Normally the user supplies the input in the form of a card deck and receives the output as a printed listing. The Prime 400 was designed primarily for interactive use, and in its current configuration it does not have an on-line card reader, so batch mode runs of the solidification model must be made from an interactive terminal. Briefly, the input parameters are specified in a card deck format, the model is run, and when execution is complete the user can view the tabulated output either on the terminal screen or in printed form. There is no graphical output from the batch mode of operation.

4.1 MAKING A BATCH RUN

The "batch" session begins with a log-in and ends with a log-out as described in Sections 3.1 and 3.6. After log-in, the user sets up an input file as described in Section 4.2. Execution of the model is invoked with the command

```
CO MPSI.BATCH
```

Execution is complete when the message OK, appears on the screen.

4.2 INPUT FILE

Input for the batch model must be set up in a facsimile of a card deck as a file in the computer mass storage. This is accomplished by using the text editor to create the input file. The text editor is thoroughly described in the Prime Corporation document "Prime Editor and Runoff", FDR3104. The input file must be stored under the name CARDS. In the input deck each data item occurs on a separate card, left justified with no embedded blanks. Number formats are discussed in Section 2.2. The first card of the data deck must contain the word "BATCH" starting in column 1, subsequent data items are the case name and the parameters described in Sections 5.2 through 5.4, in the order given there. If several cases are stacked in one run, the case name card for case M follows immediately after the last parameter card of case M-1. A sample deck is shown in Section 8.2.1. The input parameters are defined in Section 5.
4.3 VIEWING BATCH OUTPUT

The information in the batch output is described in Section 7.2 and illustrated in example 8.2.2. When execution of a batch run is complete, the output is in the mass storage file named PRINT. The user can view the output by using the text editor to display PRINT on the terminal screen, or he can make a printed copy by entering the command

```
SPOOL PRINT -FTN
```

It is a good practice to delete the PRINT file from mass storage when it is no longer of use:

```
DELETE PRINT
```

Any batch mode run will destroy a PRINT file left over from an earlier run.
Figure 4.1. Batch Mode Input Error Detection

Note: The error message is always printed immediately above the parameter in question. All input cards are scanned for errors before the run is terminated.
SECTION 5 - INPUT PARAMETERS

Described below are the parameters which define a particular case of horizontal bidirectional steady-state solidification in a casting. The same set of parameters is used in both interactive and batch modes. The default case is the case that is built-in to the interactive I/O controller: the parameters take on their default values each time interactive execution is initiated. There is no default case for a batch run: all parameters must be specified for each case. The format for the batch input cards is given in Section 4. Interactive parameter selection and modification is described in Section 3.3.

5.1 PARAMETER RANGES

The limits noted below for most parameters are used in the model only as a method of validating input. The ranges are a result of properties inherent in the definition of the model, for example $L > 0$, or of practical limitations of the numerical techniques, for example $N_x \geq 10$. Examples of range error situations for interactive and batch modes are shown in Figures 3.2 and 4.1, respectively. Not all cases that pass the range verification will produce a valid macrosegregation profile. Because the model is a system of coupled nonlinear partial differential equations, there is no a priori method of determining the actual parameter ranges in which solutions exist. If a solution does not exist for a given set of parameters, it is probable that the parameter values describe a situation that is in violation of one of the physical assumptions described in Volume I. One such situation occurs when $\gamma / E$ is sufficiently large, and it has been related to the phenomenon called freckling. The program detects freckling and terminates the calculation as shown in Figure 5.1. In other situations if a solution does not exist, the iteration on the steady-state solution will not converge.

5.2 ALLOY SPECIFICATION

The binary alloy is specified by chemical symbols denoting the solvent and solute, and a weight percent of solute. Acceptable values for these parameters depend upon the contents of the alloy data base described in Section 6 of this manual. Data describing the alloy phase diagram, the density behavior and the liquid viscosity are automatically read from the alloy data base. The default alloy is Al-4.5%Cu.
The calculation was stopped after the first iteration on $g$, because the program detected localized remelting which indicates freckle formation. Although the program logic allows display of the information computed in the first iteration, the macrosegregation profile is not valid. If the calculation had been allowed to continue, it would not have converged to a steady-state solution.
5.3 SOLIDIFICATION PROCESS PARAMETERS

The parameters in this group describe the conditions under which the casting is made including the mold geometry, the thermal conditions, and the strength of the gravitational force.

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Symbol</th>
<th>Default</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mushy zone width</td>
<td>(x_E-x_L)</td>
<td>5 cm</td>
<td>(x_E-x_L&gt;0)</td>
</tr>
<tr>
<td>Mushy zone height</td>
<td>(L)</td>
<td>10 cm</td>
<td>(L&gt;0)</td>
</tr>
<tr>
<td>Cooling rate</td>
<td>(-\frac{\partial T}{\partial t}) or (-\epsilon)</td>
<td>.396 °C/sec</td>
<td>(\epsilon&gt;0)</td>
</tr>
<tr>
<td>Gravitational force in -y direction</td>
<td>(g)</td>
<td>1 G</td>
<td>(g&gt;0)</td>
</tr>
</tbody>
</table>

5.4 PERMEABILITY MODEL PARAMETERS

The permeability model, which represents flow through a bundle of capillary tubes, is given by \(K=\gamma g^2_L\) independent of orientation. The only input parameter is \(\gamma\) with a default value \(\gamma=6 \times 10^{-7} \text{ cm}^2\) and the restriction \(\gamma>0\).

5.5 NUMERICAL METHODS CONTROL PARAMETERS

In the vast majority of cases the parameters in this group should not be changed from their default values, however operator control of these parameters could be useful in trouble-shooting. The parameters are fully explained in the discussion of numerical methods in Volume I of this report.

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Symbol</th>
<th>Default</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of horizontal mesh points</td>
<td>(N_i)</td>
<td>20</td>
<td>(10\leq N_i \leq 50)</td>
</tr>
<tr>
<td>Number of vertical mesh points</td>
<td>(N_j)</td>
<td>20</td>
<td>(10\leq N_j \leq 50)</td>
</tr>
<tr>
<td>Maximum number of pressure iterations</td>
<td>(M_{\text{sol}})</td>
<td>500</td>
<td>(M_{\text{sol}}&gt;0)</td>
</tr>
<tr>
<td>Pressure convergence criterion</td>
<td>(\epsilon_{\text{sol}})</td>
<td>(10^{-5})</td>
<td>(\epsilon_{\text{sol}}&gt;5\times10^{-6})</td>
</tr>
<tr>
<td>Maximum number of steady state iterations</td>
<td>(M_{\text{ssi}})</td>
<td>40</td>
<td>(M_{\text{ssi}}&gt;0)</td>
</tr>
<tr>
<td>Steady state convergence criterion</td>
<td>(\epsilon_{\text{ssi}})</td>
<td>(10^{-4})</td>
<td>(\epsilon_{\text{ssi}}&gt;5\times10^{-6})</td>
</tr>
</tbody>
</table>
SECTION 6 - ALLOY DATA BASE

The alloy data base contains alloy properties used by the solidification model. The use of a separate data base automatically accessed by the model frees the user from inputting relatively static alloy data with each change in mold contents, yet it allows complete flexibility in the range of alloys which can be processed. The phase diagram, density data and viscosity data for each binary system are included as well as a reference block allowing notation of data sources.

6.1 USING THE DATA BASE MANAGER

The data base exists on a disk file named M1.D.B. described in Section 6.2. The user who wants to modify or extend the data base has the choice of using the Prime text editor described in the Prime Corporation document "Prime Editor and Runoff", FDR3104, or of using the alloy data base manager described here. The data base is in card image form so that on a computer system with a card reader it could be maintained as a card deck.

The data base manager is an interactive program that controls modification and extension of the alloy data base. It gives the user the option of keeping a copy of the original data base file, but continued bookkeeping for and maintenance of such files are the responsibility of the user. The manager always assumes the file named M1.D.B., if it exists, is the old data base, and it stores the new data base under the same name. Execution of the manager program is initiated with the commands

```
CALL SEG "#MPS1.DBMGR"
```

The use of the manager to modify and extend a data base is shown in Figures 6.1 through 6.2. Operation is very similar to operation of the interactive solidification model in the input phase.

6.2 DATA BASE STRUCTURE AND FORMAT

The data base has the following card-image structure:
<table>
<thead>
<tr>
<th>CARD</th>
<th>FORMAT</th>
<th>CONTENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20A4</td>
<td>Data base identifies</td>
</tr>
<tr>
<td>2</td>
<td>A4,6X,A4,6X,2E10.3</td>
<td>Solvent, solute, minimum $C_L$, maximum $C_L$</td>
</tr>
<tr>
<td>3</td>
<td>20A4</td>
<td>5 cards for notation of data sources</td>
</tr>
<tr>
<td>4</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>&quot;</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>4E10.3</td>
<td>$dC_L/dT$, $k$, $C_E$, $T_E$</td>
</tr>
<tr>
<td>9</td>
<td>4E10.3</td>
<td>$dp_L/dC_L$, $\rho_S$, $\rho_{LE}$, $\rho_{SE}$</td>
</tr>
<tr>
<td>10</td>
<td>E10.3</td>
<td>$\mu$</td>
</tr>
</tbody>
</table>

Cards 2 through 10 are repeated for each alloy system.
Figure 6.1. Use of the Alloy Database Manager to Modify an Existing Data Set
Figure 6.2. Use of the Alloy Data Base Manager to Add New Binary System to the Data Base

6-4
SECTION 7 - OUTPUT

7.1 INTERACTIVE MODE OUTPUT

The graphical and tabular output contains enough labeling to make it self-explanatory, however a discussion of some terminology and notation may be useful. All output is labeled with the user-defined case title as well as a title line containing the alloy and the date and time of the run. Vertical variation through the mushy zone is always shown as a function of the normalized variable \( \frac{y}{L} \), where \( y \) is the distance from the bottom of the ingot and \( L \) is the ingot height. Horizontal variation across the S/L zone is shown as a function of \( \frac{(x-x_E)}{(x_L-x_E)} \) where \( x \) is distance from the chill face, \( x_L \) is distance to the liquidus isotherm, and \( x_E \) is distance to the eutectic front.

7.1.1 Graphical Output

The plot selection page shown in example 8.1.1 allows the user to choose both the function to plot and type of plot. In terms of the notation used in Volume I, the functions are defined as follows:

1. Final local average composition
   \[ \bar{c}_S \]
2. Velocity
   \[ \bar{V} \]
3. Pressure: \( P-P_0 \)
   \[ \bar{p}-p_0 \]
4. Pressure-bulk hydrostatic \( P \)
   \[ \bar{p}-p_0-p_{L_0}(L-y) \]
5. Fraction liquid
   \[ g_L \]
6. Mass flow
   \[ \rho_L g_L \bar{V} \]
7. Solute flow
   \[ \bar{c}_L \rho_L g_L \bar{V} \]

The vertical profiles are plots of variation of a function with vertical distance through the mushy zone. If the function also depends on horizontal position in the mushy zone, five vertical profiles are shown for \( \frac{(x-x_E)}{(x_L-x_E)} = 0, 0.1, 0.5, 0.9, 1 \). Similarly, the horizontal profile plots show variation of the function with horizontal distance through the mushy zone at fixed values of \( y/L \). The vector field plot shows the magnitude and direction of a two-dimensional vector at each mesh point in the mushy zone. The scale relating vector length to actual magnitude is shown in the lower left corner of the plot. All plots contain a parameter block identifying the values of the solidification process parameters and permeability model parameters used to generate the functions.
7.1.2 Tabular Output

As shown in example 8.1.1, the tabular output selection includes all the functions in the graphical output selection plus temperature, liquid composition and liquid density, $T$, $C_L$, and $\rho_L$ respectively. Items 9 and 10 are included for diagnostic purposes; the "pressure equation coefficients" are $A$ and $B$, and "local solidification rate" is

$$\frac{\partial g_L}{\partial t} = - \frac{\partial g_S}{\partial t}.$$

7.2 BATCH MODE OUTPUT

The printed output from a batch run consists of displays like those of the interactive model showing the alloy data base information used, the input parameter values, and tables of $T$, $C_L$, $\rho_L$, $g_L$, $p-p_o$, $V$, and $C_S$. In batch mode, the program does not generate graphical output. Example 8.2.2 shows the batch mode output.
SECTION 8 - SAMPLE CASES

8.1 INTERACTIVE MODE

The cases in this subsection are examples of input specification and of graphical and tabular output for interactive mode runs.

EXAMPLE 8.1.1 Default Aluminum - 4.5% Copper Case
This case is the one that the interactive model will run if no run-time changes are made to the parameter values. All input phase interaction with the model is shown. The output phase selection of plots or tabular displays is shown for the first plot and first table only.
MATERIALS PROCESSING IN SPACE
MACROSEGREGATION IN A CASTING INGOT

MODEL 1
- UNIDIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY
- STEADY STATE SOLUTION
- PLANAR ISOHERMS, RECTANGULAR MUSHY ZONE
- TEMPERATURE FIELD
- NO CONVECTION IN BULK LIQUID
- ISOTROPIC PERMEABILITY

ENTER CASE TITLE (UP TO 80 CHARACTERS)

EXAMPLE 8.1.1 - DEFAULT AL - 4.5 PCT CU CASE

ALLOY
SOLVENT: AI
SOLUTE: CU WEIGHT PERCENT: 4.50E 00
ENTER A TO CHANGE ALLOY OR P TO PROCEED.

ALLOY DATA BASE - DATA BASE REVISED 4/30/80

SOURCE OF INFORMATION FOR AL - CU
6.89E-01 TO 3.36E 01 UT. PCT. CU
DENSITIES
- R. NEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME,
  VOL 1, 1970, P 1209.
VISCOSITY
- R. NEHRABIAN, M. KEANE AND M.C. FLEMINGS, TRANS TMS-AIME,
  VOL 1, 1978, P 1209.

PHASE DIAGRAM
TEMPERATURE-COMPOSITION SLOPE
EQUILIBRIUM PARTITION RATIO
EUTECTIC COMPOSITION
EUTECTIC TEMPERATURE

DENSITIES
COMPOSITION-DENSITY SLOPE
SOLID DENSITY
LIQUID EUTECTIC DENSITY
SOLID EUTECTIC DENSITY

VISCOITY
3.80E-02 gm/(cm·sec)

ENTER P TO PROCEED
EXAMPLE 8.1.1 - DEFAULT AL - 4.5 PCT CU CASE

SOLIDIFICATION PROCESS PARAMETERS
1 MUSHY ZONE WIDTH 
2 MUSHY ZONE HEIGHT 
3 COOLING RATE 
4 GRAVITATIONAL FORCE

ENTER ITEM NUMBER TO CHANGE, OR P TO PROCEED.

EXAMPLE 8.1.1 - DEFAULT AL - 4.5 PCT CU CASE

PERMEABILITY MODEL PARAMETERS
1 GAMMA

ENTER ITEM NUMBER TO CHANGE, OR P TO PROCEED.

EXAMPLE 8.1.1 - DEFAULT AL - 4.5 PCT CU CASE

NUMERICAL METHODS CONTROL PARAMETERS
1 NUMBER OF HORIZONTAL MESH POINTS
2 NUMBER OF VERTICAL MESH POINTS
3 MAXIMUM NUMBER OF PRESSURE ITERATIONS
4 PRESSURE CONVERGENCE CRITERION
5 MAX NUMBER OF STEADY-STATE ITERATIONS
6 STEADY-STATE CONVERGENCE CRITERION

ENTER ITEM NUMBER TO CHANGE, OR P TO PROCEED.
AL 4.5000 CU SOLIDIFICATION MODEL 1 08:28:03 WED, JUN 04 1983
EXAMPLE E.1.1 - DEFAULT AL - 4.5 PCT CU CASE

ITERATION 1, (71 PRESSURE CYCLES), CONVERGENCE TEST = 1.582E-81
ITERATION 2, (59 PRESSURE CYCLES), CONVERGENCE TEST = 2.605E-82
ITERATION 3, (58 PRESSURE CYCLES), CONVERGENCE TEST = 2.250E-83
ITERATION 4, (43 PRESSURE CYCLES), CONVERGENCE TEST = 2.172E-84
ITERATION 5, (9 PRESSURE CYCLES), CONVERGENCE TEST = 2.133E-85

ENTER T TO DISPLAY TABULAR DATA,
0 TO DISPLAY GRAPHS,
8 TO TERMINATE RUN, OR
6 TO PROCEED TO NEXT CASE.

---

AL 4.5000 CU SOLIDIFICATION MODEL 1 08:28:03 WED, JUN 04 1983
EXAMPLE E.1.1 - DEFAULT AL - 4.5 PCT CU CASE

FUNCTION TO PLOT
1 FINAL LOCAL AVERAGE COMPOSITION
2 VELOCITY
3 PRESSURE: P-PH
4 PRESSURE - BULK HYDROSTATIC P
5 FRACTION LIQUID
6 MASS FLOW
7 SOLUTE FLOW

Plot type
1 VERTICAL PROFILES
2 HORIZONTAL PROFILES
3 VECTOR FIELD

ENTER ITEM NUMBER OF FUNCTION TO PLOT, OR
P TO PROCEED.
1

ENTER ITEM NUMBER OF PLOT TYPE
1

---

Minimum composition is 4.11 LT PCT CU
Minimum composition is 4.28 LT PCT CU

Automatic scaling yields plot range: 2.50 TO 6.50

Enter P to proceed with automatic scaling, or
L LOWER BOUND OF PLOT INTERVAL

8-4
VERTICAL PROFILES OF FINAL LOCAL AVERAGE COMPOSITION
EXAMPLE 8.1.1 - DEFAULT AL - 4.5 PCT CU CASE

FINAL LOCAL AVERAGE COMPOSITION (WT PCT)

<table>
<thead>
<tr>
<th>Y/L</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1.00</td>
<td>4.115E 00</td>
</tr>
<tr>
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<tr>
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<tr>
<td>0.75</td>
<td>4.715E 00</td>
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<tr>
<td>0.70</td>
<td>4.834E 00</td>
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<tr>
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<td>4.953E 00</td>
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<tr>
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<td>5.072E 00</td>
</tr>
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<tr>
<td>0.50</td>
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</tr>
<tr>
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<tr>
<td>0.40</td>
<td>5.548E 00</td>
</tr>
<tr>
<td>0.35</td>
<td>5.667E 00</td>
</tr>
<tr>
<td>0.30</td>
<td>5.786E 00</td>
</tr>
<tr>
<td>0.25</td>
<td>5.905E 00</td>
</tr>
<tr>
<td>0.20</td>
<td>6.024E 00</td>
</tr>
<tr>
<td>0.15</td>
<td>6.143E 00</td>
</tr>
<tr>
<td>0.10</td>
<td>6.262E 00</td>
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<tr>
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<td>6.381E 00</td>
</tr>
<tr>
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<td>6.499E 00</td>
</tr>
</tbody>
</table>

ORIGINAL PAGE IS
OF POOR QUALITY
EXAMPLE 8.1.2 ZERO GRAVITY CASE

All parameters except the gravitational force are the same as in example 8.1.1. The procedure for changing an input parameter is shown below. The resulting final composition profile and velocity field are shown on the following pages.
VERTICAL PROFILES OF
FINAL LOCAL AVERAGE COMPOSITION
EXAMPLE 8.1.3 TIN - 15% LEAD CASE

The alloy specification procedure is shown below. The numerical methods control parameters have the default values shown in example 8.1.1. All other parameter values are shown on the plots.

ALLOY

SOLVENT: AL
SOLUTE: CU
WEIGHT PERCENT: 4.50E-0

ENTER A TO CHANGE ALLOY OR P TO PROCEED.

ENTER SOLVENT (UP TO 4 CHARACTERS)
SN
ENTER SOLUTE (UP TO 4 CHARACTERS)
Pb
ENTER WEIGHT PERCENT
15

ALLOY DATA BASE - DATA BASE REVISED 4/30/88

SOURCE OF INFORMATION FOR SN - Pb
8.88E-01 TO 3.81E-01 WT. PCT. Pb

PHASE DIAGRAM - METALS HANDBOOK, VOL 8, ASM, 1973, P278.


PHASE DIAGRAM
TEMPERATURE-COMPOSITION SLOPE
-7.75E-01 PCT SOLUTE / DEG C
EQUILIBRIUM PARTITION RATIO
6.56E-02
EUTECTIC COMPOSITION
3.81E-01 PCT SOLUTE
EUTECTIC TEMPERATURE
1.89E 02 DEG C

DENSITIES
COMPOSITION-DENSITY SLOPE
3.27E-02 (GM/CM3#13) / PCT SOLUTE
SOLID DENSITY
7.30E 00 GM/CM3
LIQUID EUTECTIC DENSITY
8.19E 00 GM/CM3
SOLID EUTECTIC DENSITY
8.59E 00 GM/CM3

VISCOITY
2.20E-02 CN/(CM SEC)

ENTER P TO PROCEED
Vertical Profiles of Final Local Average Composition
SOLIDIFICATION MODEL 1
EXAMPLE 8.1.3  T1M - 15 PCT LEAD CASE
08:42/11 WED, JUN 04 1980

VELOCITY FIELD
SCALE: 9.278E-03 (CM/SEC)

XL=NE 5.0 CM
L= 6.3 CM
GAMMA= 5.00E-87
G= 5.04 DEG C/CM
EPS= -0.508 DEG/SEC
GRAVITY= 1.00 G
EXAMPLE 8.1.4  TIN - 3% BISMUTH CASE

The alloy specification procedure is shown below. The numerical methods control parameters have the default values shown in example 8.1.1. All other parameter values are shown on the plots.

ALLOY

SOLVENT:  SN
SOLUTE:  Pb  WEIGHT PERCENT:  1.588E+01

ENTER A TO CHANGE ALLOY OR P TO PROCEED.
A
......ENTER SOLVENT (UP TO 4 CHARACTERS)
SN
......ENTER SOLUTE (UP TO 4 CHARACTERS)
Pb

ENTER WEIGHT PERCENT
3

ALLOY DATA BASE  -  DATA BASE REvised 4/30/80

SOURCE OF INFORMATION FOR SN - Pb
6.89E-01 TO 6.99E-01 WT. PCT. Pb
PHASE DIAGRAM - METALS HANDBOOK, VOL 8, ASM, 1973,
DENSITIES  - D.R. POIRIER (APPENDIX A, VOL II, FPS SOLIDIFICATION
MODEL FORMULATION AND ANALYSIS)
DENSITIES  - D.R. POIRIER (APPENDIX A, VOL II, FPS SOLIDIFICATION
MODEL FORMULATION AND ANALYSIS)

PHASE DIAGRAM

TEMPERATURE-COMPOSITION SLOPE  -6.382E-01 PCT SOLUTE / DEG C
EQUILIBRIUM PARTITION RATIO  3.233E-01
EUTECTIC COMPOSITION  6.89E-01 PCT SOLUTE
EUTECTIC TEMPERATURE  1.388E+02 DEG C

DENSITIES

COMPOSITION-DENSITY SLOPE  2.773E-02 (GM/CM**3) / PCT SOLUTE
SOLID DENSITY  7.242E+00 GM/CM**3
LIQUID EUTECTIC DENSITY  8.652E+00 GM/CM**3
SOLID EUTECTIC DENSITY  8.688E+00 GM/CM**3

VISCOOSITY  2.152E-02 GR/(CM**5SEC)

ENTER P TO PROCEED
VERTICAL PROFILES OF FINAL LOCAL AVERAGE COMPOSITION
8.2 BATCH MODE

The batch mode input is in the form of a card deck or a disk file in card image format, and the output is limited to a printed listing. The card deck for running the batch equivalent of example 8.1.1 is shown below. The output generated by running the model with this input deck is in subsection 8.2.2.

8.2.1 Input Deck, Aluminum - 4.5% Copper Case

All entries begin in column 1.
8.2.2 Printed Output

MATERIALS PROCESSING IN SPACE
MACROSEGREGATION IN A CASTING INGOT

MODEL 1
- UNIDIRECTIONAL SOLIDIFICATION OF A BINARY ALLOY
- STEADY STATE SOLUTION
- PLANAR ISOTHERMS, RECTANGULAR MUSHY ZONE
- TEMPERATURE FIELD INPUT
- NO CONVECTION IN BULK LIQUID
- ISOTROPIC PERMEABILITY X = GAMMA

AL 4.5000 CU SOLIDIFICATION MODEL 1 09/19/83 WED, JUN 04 1989
EXAMPLE 8.2 - BATCH ALUMINUM - 4.5 PCT COPPER CASE

ALLOY DATA BASE - DATA BASE REVISED 4/28/88

SOURCE OF INFORMATION FOR AL - CU
8.000E-01 TO 3.330E 01 WT. PCT. CU
PHASE DIAGRAM - M.C. FLEMINGS AND W. KEREN, MET TRANS, VOL 239, 1967, P 1449.
DENSITIES - R. MEHRABIAN, M. KERNE AND M.C. FLEMINGS, TRANS TMS-AIME,
VOL 1, 1979, P 1299.
VISCOSITY - R. MEHRABIAN, M. KERNE AND M.C. FLEMINGS, TRANS TMS-AIME,
VOL 1, 1979, P 1299.

PHASE DIAGRAM
TEMPERATURE-COMPOSITION SLOPE -2.88E-01 PCT SOLUTE / DEG C
EQUILIBRIUM PARTITION RATIO 1.72E-01
EUTECTIC COMPOSITION 3.30E-01 PCT SOLUTE
EUTECTIC TEMPERATURE 5.40E-02 DEG C

DENSITIES
COMPOSITION-DENSITY SLOPE 2.67E-02 (GM/CM^3) / PCT SOLUTE
SOLID DENSITY 2.62E00 GM/CM^3
LIQUID EUTECTIC DENSITY 3.22E00 GM/CM^3
SOLID EUTECTIC DENSITY 3.40E00 GM/CM^3

VISCOSITY
3.00E-02 GM/(CM^SEC)

AL 4.5000 CU SOLIDIFICATION MODEL 1 09/19/83 WED, JUN 04 1989
EXAMPLE 8.2 - BATCH ALUMINUM - 4.5 PCT COPPER CASE

CASE INPUT

SOLIDIFICATION PROCESS PARAMETERS
1 MUSHY ZONE WIDTH 5.00E-02 (CM)
2 MUSHY ZONE LENGTH 1.00E-01 (CM)
3 COOLING RATE 3.00E-01 (DEG C/SEC)
4 GRAVITATIONAL FORCE 1.00E-02 (G)

PERMEABILITY MODEL PARAMETERS
1 GAMMA 6.00E-07 (CM^2)

NUMERICAL CONTROL PARAMETERS
1 NUMBER OF HORIZONTAL MESH POINTS 20
2 NUMBER OF VERTICAL MESH POINTS 20
3 MAXIMUM NUMBER OF PRESSURE ITERATIONS 500
4 PRESSURE CONVERGENCE CRITICAL 1.00E-05
5 MAX NUMBER OF STEADY-STATE ITERATIONS 40
6 STEADY-STATE CONVERGENCE CRITICAL 1.00E-04
(This section consists of tables of $T$, $C_L$, $\rho_L$, $g_L$, $p-p_o$, and $\vec{v}$ in a format identical to the tabular output from an interactive mode case.)

---

**AL 4.5000 CU SOLIDIFICATION MODEL 1 09:19:13 WED, JUN 04 1981**

**EXAMPLE 8.2 - BATCH ALUMINUM - 4.5 PCT COPPER CASE**

**FINAL LOCAL AVERAGE COMPOSITION (UT PCT)**

<table>
<thead>
<tr>
<th>$\sqrt{L}$</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
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</tbody>
</table>

***** NORMAL TERMINATION